Condensed Matter Physics II. – A.A. 2015-2016, April 29, 2016

(*time 3 hours*)

Solve the following two exercises.

NOTE:

- Give all details which help in understanding the proposed solution. Answers which only contain the final result or not enough detail will be judged insufficient and discarded;
- If you are requested to give evaluation/estimates, do so using 3 significant figures.

Exercise 1: *LDA (with exchange) for a 1D electron gas*

Consider Fermions of spin 1/2 in 1D with a pair interaction that using the Ry and a_B as units of energy and length respectively, reads $2\delta(x_1 - x_2)$ are under the action of an external potential $v(x)$. In HF the energy per particle reads:

$$\epsilon(\rho) = \frac{A}{3}\rho^2 - \frac{1}{2}\rho$$

where $\rho = N/L$, the Fermions are spin unpolarized, and the first and second term are respectively the kinetic energy end the exchange energy per particle. In the following neglect the correlation energy. The constant appearing above has the simple expression $A = (\pi/2)^2$.

1. Write in LDA the internal energy functional (kinetic + exchange energies only!).
2. Using the result above, write the full energy functional (kinetic + exchange energies + interaction with external potential) and impose the extremum condition.
3. Use the extremum condition to obtain an expression for $\rho(x)$. As you should have got a quadratic equation you should have two solutions.
4. In order to select solutions that correspond to a minimum you need to take the second functional derivative. Note that, if the second functional derivative has the form $g(\rho(x))\delta(x - x')$, it is easy to show that a sufficient condition for a minimum is $g(\rho(x)) > 0$ for all values of x, apart from a set of null measure in the x domain (isolated points in 1D).
5. Give the expression of the equilibrium $\rho(x)$ when

   $$\pi^2 v(x) = 1 - [sin(x)]^2, \quad \pi^2\mu = c^2,$$

   and c is real.
6. Provide qualitative skecthes of $v(x)$ and of $\rho(x)$ when $c = 0$ and $c >> 1$.

Exercise 2: *Effective masses in a semiconductor*

The experimental analysis of a certain semiconductor shows that the density of states in energy of a specific band has, close to the band edge $\mathbf{k}^*$ of that band, the expected square root behaviour $g(\epsilon) = C\sqrt{\epsilon}$, where $\epsilon = |E - E^*|$ and $C = 1.01 \times 10^{39}\, cm^{-3} erg^{-3/2}$. In what follows we shall assume that the laboratory coordinate system coincides with the principal axes system ($\hat{x}_1$, $\hat{x}_2$, $\hat{x}_3$) of the mass tensor at $\mathbf{k}^*$.

1. How much is the determinant of the mass tensor in units of m_e^3?
2. Performing experiments in a magnetic field one finds that rotating $\mathbf{H}$ around the $\hat{x}_3$ axis the cyclotron effective mass does not change. How many different eigenvalues has, at most, the mass tensor? Argue your answer in full details. You may use $\hat{\mathbf{H}} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)$ to realize that the mentioned rotation amounts to vary ϕ between 0 and 2π.
3. Knowing that for a magnetic field orthogonal to the $\hat{x}_3$ axis the cyclotron mass is $m^*(\mathbf{H}) = 0.469 m_e$ compute the eigenvalues of the mass tensor (in units of m_e).
4. What is the shape of the orbits for a magnetic field lying along the $\hat{x}_3$ axis?
5. And for a magnetic field lying along the $\hat{x}_1$ axis?
6. What will be the measured cyclotron frequency (in cm^{-1}) for a magnetic field with $\hat{H} = (1/\sqrt{2}, 0, 1/\sqrt{2})$ and H=1 gauss?